Robust PDE Constrained Optimization with Multilevel Monte Carlo Methods

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Overview

1. Robust control problem
2. Optimality conditions
3. Effect of the variance estimator
4. Multilevel Monte Carlo sampling
5. Optimization with uncertainties
6. Numerical results

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Robust control problem

Deterministic problem

$$\min_{y,u} \quad J_{\text{det}}(y,u) \ \text{ s.t. } \quad c(y,u,k) = 0$$

Robust control problem

$$\min_{y,u} \quad J(y,u) = \mathbb{E}[J_{\text{det}}(y,u)] + \gamma \|\mathbb{S}[y]\|^2 \ \text{ s.t. } \quad c(y,u,k) = 0$$

$\gamma > 0$ and J_{det} convex $\Rightarrow$ J convex

Note: Other risk measures exist

Common case: tracking target y_D

$$\begin{aligned} J(y,u) &= \mathbb{E}[\|y - y_D\|^2] + \alpha\|u\|^2 + \gamma\|\mathbb{S}[y]\|^2 \\ &= \|\mathbb{E}[y] - y_D\|^2 + \alpha\|u\|^2 + (\gamma+1)\|\mathbb{S}[y]\|^2 \end{aligned}$$

Equivalence of robust and average control for 2-norm tracking

$\gamma > -1 \Rightarrow J$ convex and quadratic

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Optimality conditions

Lagrangian $\mathcal{L}(y,u,p) = J(y,u) + (p, c(y,u,k))$

$$\begin{cases} \nabla_p \mathcal{L} = 0 \\ \nabla_y \mathcal{L} = 0 \\ \nabla_u \mathcal{L} = 0 \end{cases} \Rightarrow \begin{cases} 0 = c(y,u) & \leftarrow \text{constraint equation} \\ 0 = \left(\dfrac{\partial c}{\partial y}\right)^* [p] + \nabla_y J & \leftarrow \text{adjoint equation} \\ 0 = \left(\dfrac{\partial c}{\partial u}\right)^* [p] + \nabla_u J = \nabla \tilde{J}(u) \end{cases}$$

$\tilde{J}(u)$ is the reduced cost functional (y eliminated using c)

If $J(y,u) = \mathbb{E}[J_{\text{det}}(y,u)] + \gamma \|\mathbb{S}[y]\|^2$

$$\begin{cases} c(y,u) = 0 \\ -\left(\dfrac{\partial c}{\partial y}\right)^* [p] = \nabla_y J_{\text{det}} + 2\gamma(y - \mathbb{E}[y]) \\ \nabla \tilde{J}(u) = \left(\dfrac{\partial c}{\partial u}\right)^* [p] + \mathbb{E}[\nabla_u J_{\text{det}}] = 0 \end{cases}$$

Optimality conditions

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Estimating $\mathbb{E}[\nabla_u J_{\mathsf{det}}]$ using (ML)MC requires estimating $\mathbb{E}[y]$ first

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Estimators for the variance $\mathbb{V}[y]$

Let Ω be the set of all possible random realizations ω
(k and y depend on ω)

- Estimator $\hat{V}[y]$ using samples $\Omega_0 \subset \Omega$

$$\hat{V}_0[y] \triangleq \frac{1}{n}\sum_{j=1}^{n}(y_j - \frac{1}{n}\sum_{i=1}^{n} y_i)^2$$

$$\nabla_y \left\| \sqrt{\hat{V}_0[y]} \right\|^2 = 2(y - \frac{1}{n}\sum_{i=1}^{n} y_i)$$

(proof: $\nabla_y \|\mathbb{S}[y]\|^2 = \gamma(y - \mathbb{E}[y])$ holds for any stochastic space, and therefore also for a finite subset of n equally probable samples $\Omega_0 \subset \Omega$ $\square$)

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Using $\hat{V}[y]$ corresponds to using MC estimator for $\mathbb{E}[y]$

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Using $\hat{V}[y]$ corresponds to using MC estimator for $\mathbb{E}[y]$

Problems: - Either large memory required or double work
- Which accuracy to request for $\mathbb{E}[y]$?

Estimators for the variance $\mathbb{V}[y]$

Let Ω be the set of all possible random realizations ω (k and y depend on ω)

- Another estimator $\hat{V}'[y]$ also using samples $\Omega_0 \subset \Omega$

$$\hat{V}'[y] \triangleq \frac{1}{2n} \sum_{j=1}^{n} (y_j - y_{j-1})^2$$

$$\nabla_y \left\| \sqrt{\hat{V}'[y]} \right\|^2 = 2y - y_{+1} - y_{-1}$$

The j-th sample is $\gamma(2y_j - y_{j+1} - y_{j-1})$ with $y_{n+i} = y_i$

$\hat{V}'[y]$ is an unbiased estimator for $\mathbb{V}[y]$
(proof: $\mathbb{E}[(y_j - y_{j-1})^2] = \mathbb{E}[(y_j - \mathbb{E}[y] + \mathbb{E}[y] - y_{j-1})^2] = \mathbb{E}[(y_j - \mathbb{E}[y])^2] + \mathbb{E}[(\mathbb{E}[y] - y_{j-1})^2] = 2\mathbb{V}[y]$ $\square$)

Estimators for the variance $\mathbb{V}[y]$

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(+) No more $\mathbb{E}[.]$ required in advance.
(-) Samples are no longer independent!
(-) RMSE($\hat{V}'[y]$) $= 1.5 \cdot$ RMSE($\hat{V}[y]$).

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Multilevel Monte Carlo Sampling

Assume a quantity of interest Q (e.g., point value of p)

Multilevel Monte Carlo idea

- Multiple discretization levels $m_0 < m_1 < \ldots < m_L$
- Multiple approximations $Q_{m_0}, \ldots, Q_{m_L}$ for Q
- Telescopic sum

$$\mathbb{E}[Q_{m_L}] = \mathbb{E}[Q_{m_0}] + \sum_{\ell=1}^{L} \mathbb{E}[Q_{m_\ell} - Q_{m_{\ell-1}}] = \sum_{\ell=0}^{L} \mathbb{E}[Y_\ell]$$

Multilevel Monte Carlo estimator

$$\hat{Q}_{\boldsymbol{m},\boldsymbol{n}}^{\mathsf{MLMC}} \triangleq \sum_{\ell=0}^{L} \hat{Y}_{\ell,n_\ell}^{\mathsf{MC}} \quad \text{with} \quad \hat{Y}_{\ell,n_\ell}^{\mathsf{MC}} = \frac{1}{n_\ell} \sum_{i=1}^{n_\ell} \Big(Q_{m_\ell}(\omega_i) - Q_{m_{\ell-1}}(\omega_i) \Big)$$

Multilevel Monte Carlo Sampling

Mean Square Error

$$\mathbb{E}\Big[\big(\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}} - \mathbb{E}[Q]\big)^2\Big] = \underbrace{\mathbb{V}[\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}}]}_{\text{stochastic error}} + \underbrace{(\mathbb{E}[Q_{m_L}] - \mathbb{E}[Q])^2}_{\text{bias = discretization error}} \leq \epsilon^2$$

Independent samples

$$\mathbb{V}[\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}}] = \sum_{\ell=0}^{L} \mathbb{V}[\hat{Y}^{\mathsf{MC}}_{\ell,n_\ell}] = \sum_{\ell=0}^{L} n_\ell^{-1}\mathbb{V}[Y_\ell]$$

- Amount of levels L incremented until bias (estimated) is small enough.
- Amount of samples $\boldsymbol{n} = (n_0, n_1, \ldots, n_L)$ chosen such that stochastic error is small enough.

Multilevel Monte Carlo Sampling

Mean Square Error

$$\mathbb{E}\left[\left(\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}} - \mathbb{E}[Q]\right)^2\right] = \underbrace{\mathbb{V}[\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}}]}_{\text{stochastic error}} + \underbrace{(\mathbb{E}[Q_{m_L}] - \mathbb{E}[Q])^2}_{\text{bias} = \text{discretization error}} \leq \epsilon^2$$

Dependent samples

$$\mathbb{V}[\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}}] = \sum_{\ell=0}^{L} \mathbb{V}[\hat{Y}^{\mathsf{MC}}_{\ell,n_\ell}] = \sum_{\ell=0}^{L} n_\ell^{-2} \sum_{i=1}^{n_\ell} \sum_{j=1}^{n_\ell} \mathsf{Cov}[Y_{\ell,i}, Y_{\ell,j}]$$

- Amount of levels L incremented until bias (estimated) is small enough.
- Amount of samples $\boldsymbol{n} = (n_0, n_1, \ldots, n_L)$ chosen such that stochastic error is small enough.

Multilevel Monte Carlo Sampling

Mean Square Error

$$\mathbb{E}\Big[\big(\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}} - \mathbb{E}[Q]\big)^2\Big] = \underbrace{\mathbb{V}[\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}}]}_{\text{stochastic error}} + \underbrace{(\mathbb{E}[Q_{m_L}] - \mathbb{E}[Q])^2}_{\text{bias } = \text{ discretization error}} \leq \epsilon^2$$

Dependent samples (circulant covariance matrix)

$$\mathbb{V}[\hat{Q}^{\mathsf{MLMC}}_{\boldsymbol{m},\boldsymbol{n}}] = \sum_{\ell=0}^{L} \mathbb{V}[\hat{Y}^{\mathsf{MC}}_{\ell,n_\ell}] = \sum_{\ell=0}^{L} n_\ell^{-1} \Big(\mathbb{V}[Y_\ell] + 2 \sum_{j=2}^{b+1} \mathsf{Cov}[Y_{\ell,1}, Y_{\ell,j}]\Big)$$

- Amount of levels L incremented until bias (estimated) is small enough.
- Amount of samples $\boldsymbol{n} = (n_0, n_1, \ldots, n_L)$ chosen such that stochastic error is small enough.

Multilevel Monte Carlo Sampling

Theorem (MLMC cost[1])

Assumptions *(slightly simplified)*

$$|\mathbb{E}[Q_{m_\ell} - Q]| \lesssim m_\ell^{-\rho} \qquad \mathbb{V}[Y_\ell] \lesssim m_\ell^{-\phi} \qquad \mathcal{C}_\ell \lesssim m_\ell^{\kappa}$$

MLMC cost

$$\mathcal{C}_{MLMC}(\epsilon) \lesssim \begin{cases} \epsilon^{-2} & \text{if } \phi > \kappa \\ \epsilon^{-2}(\log \epsilon)^2 & \text{if } \phi = \kappa \\ \epsilon^{-2-(\kappa-\phi)/\rho} & \text{if } \phi < \kappa \end{cases}$$

For dependent samples: replace $\mathbb{V}[Y_\ell]$ as suggested by the previous slides. Note: in the last case, no amendmend is needed since

$$\mathbb{V}[Y_\ell] \lesssim m_\ell^{-\phi} \Rightarrow \mathbb{V}[Y_\ell] + 2\sum_{j=2}^{b+1} \mathrm{Cov}[Y_{\ell,1}, Y_{\ell,j}] \lesssim m_\ell^{-\phi}$$

[1] K. A. Cliffe, M. B. Giles, R. Scheichl, *Multilevel Monte Carlo methods and applications to elliptic PDEs with random coefficients*, Computing and Visualization in Science, vol. 14(1), pp. 3–15, 2011.

Model problem

Classical model problem

- Diffusion PDE constraint $c(y,u,k)=0$

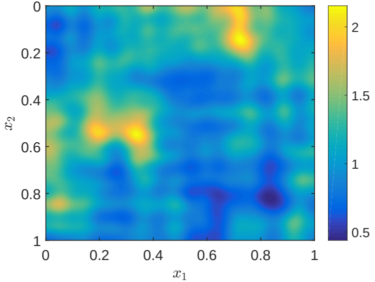
$$\begin{aligned} -\nabla\cdot(k(x,\omega)\nabla y(x,\omega)) &= u(x) \quad \text{on } D\\ y(x,\omega) &= 0 \qquad \text{on } \partial D \end{aligned}$$

- lognormal random field $k(x,\omega)=\exp(z(x,\omega))$ with z Gaussian. $\mathbb{E}[z(x,\omega)]=0$ and, e.g.,

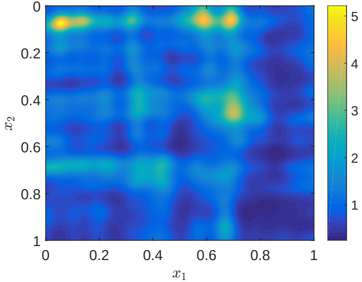
$$\mathrm{Cov}(z(x_1,\omega),z(x_2,\omega))=\sigma^2\exp\left(-\frac{\|x_1-x_2\|_1}{\lambda}\right)$$

- Robust tracking type cost: $\mathbb{E}[\|y-y_D\|^2]+\alpha\|u\|^2+\gamma\|\mathbb{S}[y]\|^2$

Samples of k



(a) $\sigma^2 = 0.1,\ \lambda = 0.3$



(b) $\sigma^2 = 0.5,\ \lambda = 0.3$

generated using, e.g., the KL-expansion or circulant embedding

Optimality conditions, gradient and Hessian

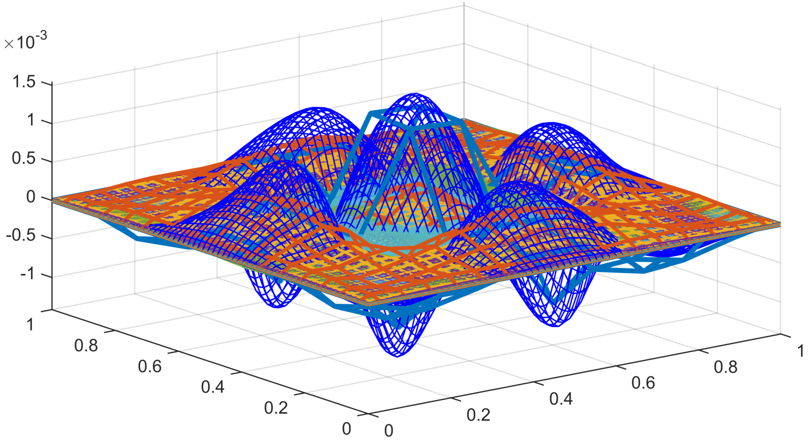
Gradient: $\nabla \tilde{J}(u)$

$$\left\{ \begin{array}{rcl} -\nabla \cdot (k \nabla y) & = & u \\ -\nabla \cdot (k \nabla p) & = & 2(y - y_D) + 2\gamma(y - \mathbb{E}[y]) \\ \nabla \tilde{J}(u) & = & 2\alpha u + \beta \mathbb{E}[p] \end{array} \right.$$

Hessian: Hess $\tilde{J}(u)[\delta u]$

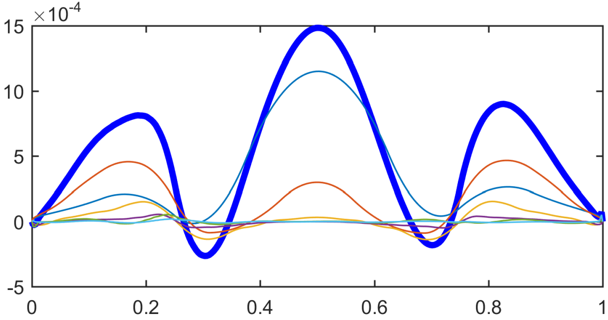
$$\left\{ \begin{array}{rcl} -\nabla \cdot (k \nabla\, \delta y) & = & \delta u \\ -\nabla \cdot (k \nabla\, \delta p) & = & 2\, \delta y + 2\gamma(\delta y - \mathbb{E}[\delta y]) \\ \text{Hess } \tilde{J}(u)[\delta u] & = & 2\alpha\, \delta u + \mathbb{E}[\delta p] \end{array} \right.$$

Multilevel decomposition of gradient



Multilevel decomposition of gradient

Cross section of gradient contributions after mapping to the finest level.



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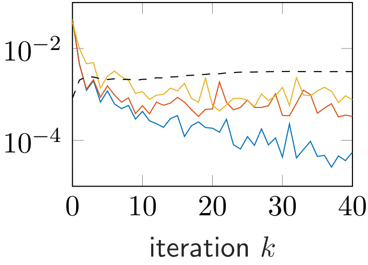
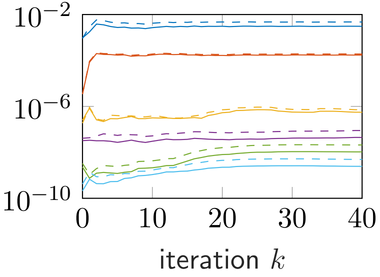
Behavior of optimization and evolution of variances





(a) $\|\nabla \hat{J}_f(\boldsymbol{u}_f^{(k)})\|$ (——), $\|\nabla \hat{J}_\$(\boldsymbol{u}_f^{(k)})\|$ (——), $\|\nabla \hat{J}_\$(\boldsymbol{u}_\$^{(k)})\|$ (——), RMSE ϵ of $\nabla \hat{J}_f(\boldsymbol{u}_f^{(k)})$ (- - -).

(b) $\|\mathbb{V}[\boldsymbol{Y}_\ell]\|_\infty$ (- - -), $\|\max\{\frac{1}{2}\mathbb{V}[\boldsymbol{Y}_\ell], \mathbb{V}[\boldsymbol{Y}_\ell] + 2\sum_{j=2}^{b+1} \mathsf{Cov}[\boldsymbol{Y}_{\ell,1}, \boldsymbol{Y}_{\ell,j}]\}\|_\infty$ (——) for levels $\ell = \{0, \ldots, 5\}$.

Convergence behaviour

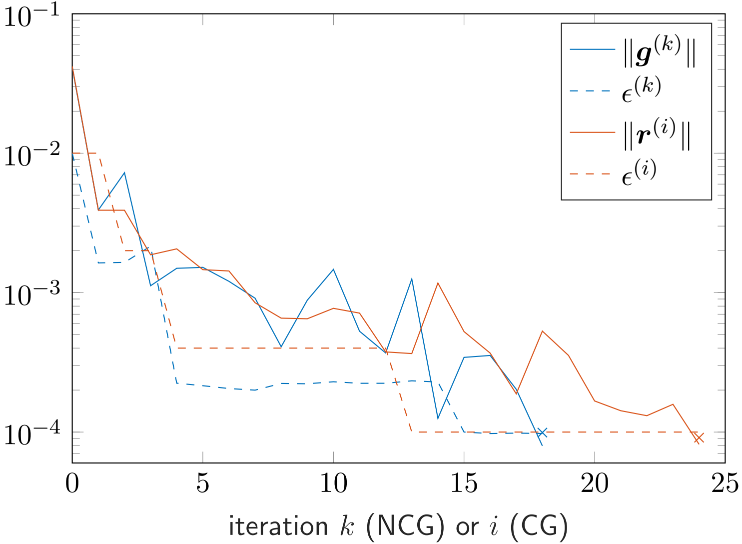


Figure: Behavior of gradient (NCG) and Hessian (CG) based optimization

MLMC optimization cost

Theorem (MLMC optimization cost)

Assumptions *Same assumptions but uniformly in an area of the optimal point* $\bar{u}$ *and uniformly for each point of the gradient:*

$$|\mathbb{E}[Q_{m_\ell} - Q]| \lesssim m_\ell^{-\rho} \qquad \mathbb{V}[Y_\ell] \lesssim m_\ell^{-\phi} \qquad \mathcal{C}_\ell \lesssim m_\ell^{\kappa}$$

Optimization cost *(using the gradient or Hessian based algorithm) to reach gradient norm* τ

$$\mathcal{C}_{opt}(\tau) \lesssim \begin{cases} \tau^{-2} & \text{if } \phi > \kappa \\ \tau^{-2}(\log \tau)^2 & \text{if } \phi = \kappa \\ \tau^{-2-(\kappa-\phi)/\rho} & \text{if } \phi < \kappa \end{cases}, \quad \tau \to 0. \tag{1}$$

Again, for dependent samples, replace $\mathbb{V}[Y_\ell]$ *as suggested by the previous slides.*

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Example 1

problem description		solver parameters	
$\alpha = 1\text{e}{-6}$	$\sigma^2 = 0.1$	$m_0 = 8$	$\bar{L} = 5$
$\gamma = 1$	$\lambda = 0.3$	$m_{\bar{L}} = 256$	$\mathsf{TOL} = 1\text{e}{-4}$

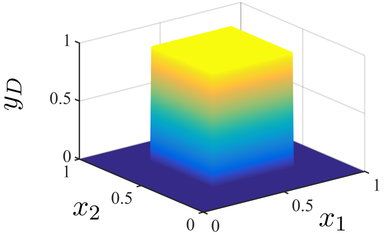


Figure: Target function y_D.

Example 1

Gradient based algorithm:

Total time: 1542s

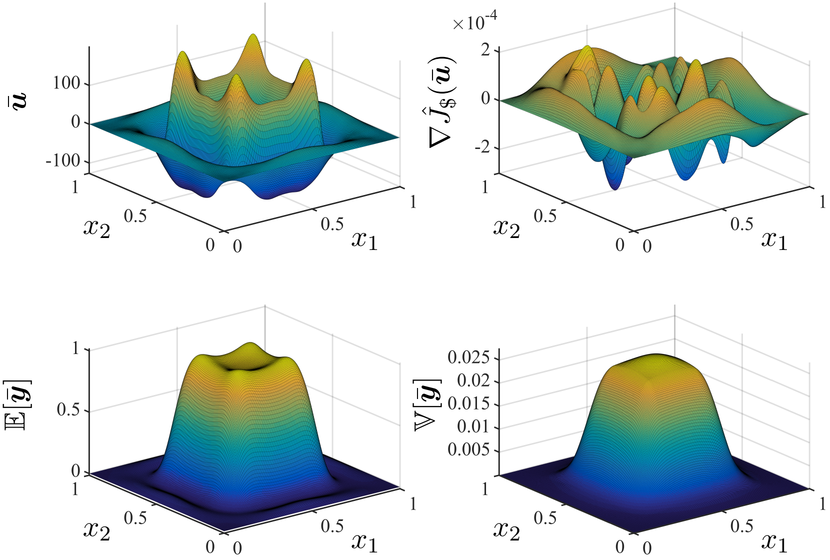
k	$\epsilon^{(k)}$	n_0	n_1	n_2	n_3	n_4	n_5	estimate of ρ	$t^{(k)}$
0	0.01	140	76	44				2.0237	2.05
4	2.24e−4	17150	1512	80	28	20		1.5824	47.49
15	1e−4	98452	9156	940	118	20		1.5825	248.84

Hessian based algorithm:

Total time: 1989s

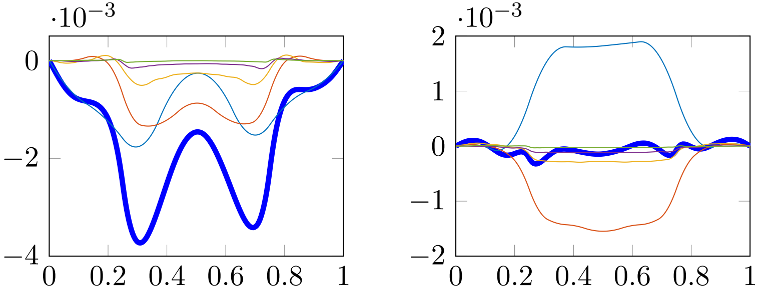
i	$\epsilon^{(i)}$	n_0	n_1	n_2	n_3	n_4	n_5	estimate of ρ	$t^{(k)}$
0	0.01	140	76	44				1.8355	8.25
2	2e−3	140	76	44				1.703	8.73
4	4e−4	5964	521	44	28	20		1.5905	130.11
13	1e−4	96159	9010	821	93	22		1.6195	1841.44

Example 1



$\bar{\boldsymbol{u}}$
100
0
-100
1
0.5
0
x_2
0
0.5
1
x_1
$\times 10^{-4}$
2
0
-2
$\nabla \hat{J}_{\$}(\bar{\boldsymbol{u}})$
$\mathbb{E}[\bar{\boldsymbol{y}}]$
1
0.5
0
$\mathbb{V}[\bar{\boldsymbol{y}}]$
0.025
0.02
0.015
0.01
0.005

Example 1



(a) Iteration $k = 5$ (b) Iteration $k = 18$ (last)

Figure: Cross section of $\boldsymbol{g}^{(k)} = \sum_{\ell=0}^{L} I_\ell^{\bar{L}} \hat{Y}_{\ell,n_\ell}^{\mathsf{MC}}$ (——) and contributions $I_\ell^{\bar{L}} \hat{Y}_{\ell,n_\ell}^{\mathsf{MC}}$ for levels $0, \ldots, L$ (——, ——, ——, ——, ——).

Example 2

problem description		solver parameters	
$\alpha = 1\text{e}{-5}$	$\sigma^2 = 0.5$	$m_0 = 8$	$\bar{L} = 5$
$\gamma = 0$	$\lambda = 0.3$	$m_{\bar{L}} = 256$	$\mathsf{TOL} = 1\text{e}{-4}$

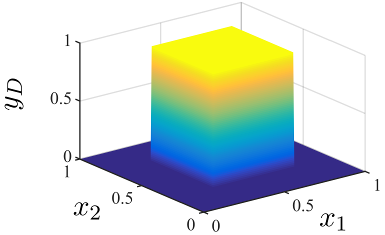


Figure: Target function y_D.

Example 2

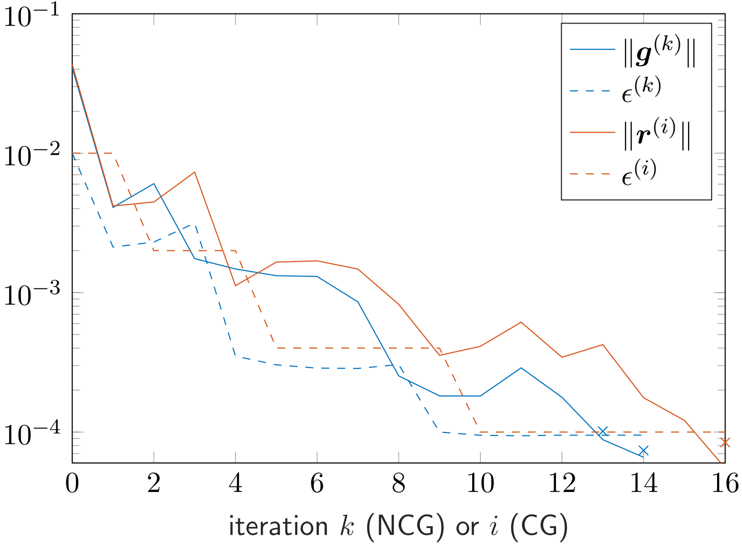


Figure: Behavior of gradient (NCG) and Hessian (CG) based optimization

Example 2

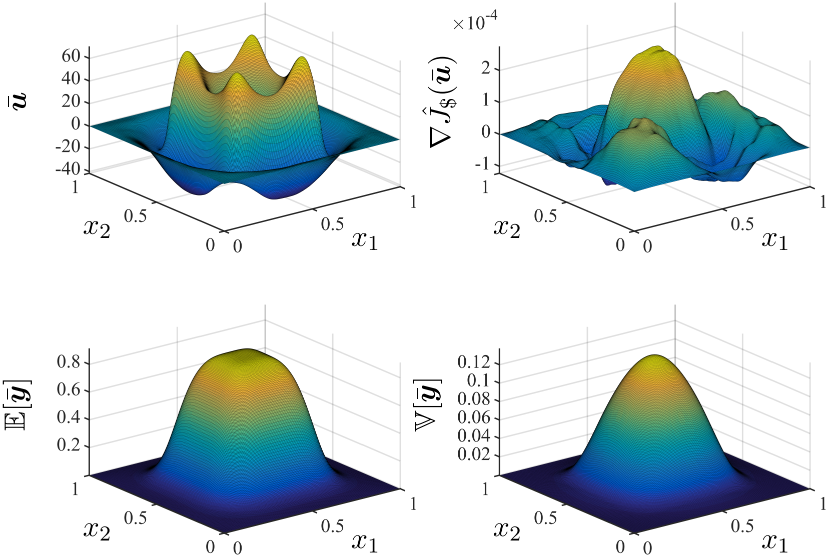
Gradient based algorithm: Total time: 6973s

k	$\epsilon^{(k)}$	n_0	n_1	n_2	n_3	n_4	n_5	estimate of ρ	$t^{(k)}[s]$
0	0.01	140	76	44				2.0237	2.06
4	3.51e−4	35563	3220	136	28	20		1.5824	93.44
9	1e−4	375256	38259	2082	135	21	16	1.5825	1092.71

Hessian based algorithm: Total time: 5114s

i	$\epsilon^{(i)}$	n_0	n_1	n_2	n_3	n_4	n_5	estimate of ρ	$t^{(i)}[s]$
0	0.01	140	76	44				1.9102	8.89
2	2e−3	393	76	44				2.0975	11.77
5	4e−4	33063	6980	193	28	20		1.7029	76.20
10	1e−4	388834	37023	1747	255	56	16	1.7818	668.58

Example 2



$\bar{\boldsymbol{u}}$
60
40
20
0
-20
-40
x_2
x_1
0
0.5
1
$\times 10^{-4}$
$\nabla \hat{J}_{\$}(\bar{\boldsymbol{u}})$
2
1
0
-1
$\mathbb{E}[\bar{\boldsymbol{y}}]$
0.8
0.6
0.4
0.2
$\mathbb{V}[\bar{\boldsymbol{y}}]$
0.12
0.1
0.08
0.06
0.04
0.02

Example 3

problem description		solver parameters	
$\alpha = 1\text{e}{-6}$	$\sigma^2 = 0.1$	$m_0 = 16$	$\bar{L} = 5$
$\gamma = 5$	$\lambda = 0.3$	$m_{\bar{L}} = 512$	$\mathsf{TOL} = 5\text{e}{-5}$

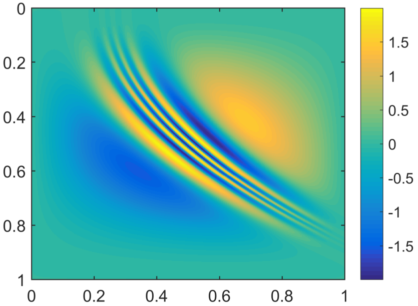
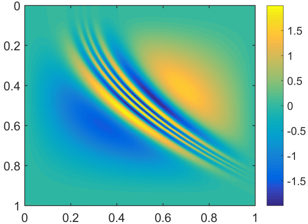
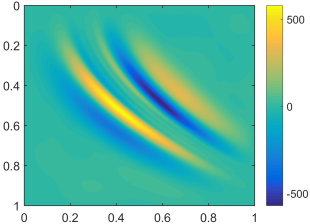


Figure: Target function y_D.

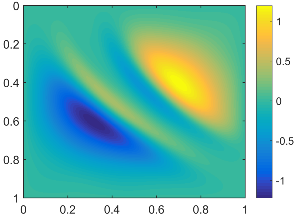
Example 3



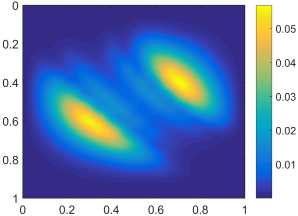
(a) target $\boldsymbol{y}_D$.



(b) Calculated optimum $\bar{\boldsymbol{u}}$.

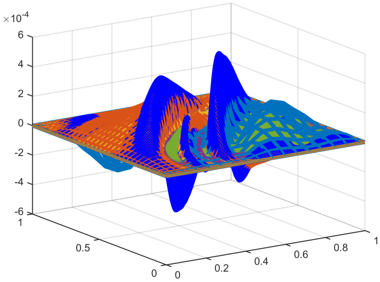


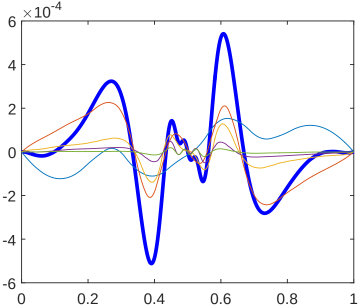
(c) $\mathbb{E}[\bar{\boldsymbol{y}}]$.



(d) $\mathbb{V}[\bar{\boldsymbol{y}}]$.

$\bar{\boldsymbol{p}}$ at the solution





Test using new samples: $\|\nabla \tilde{J}_{\$}(\bar{\boldsymbol{u}})\| = 5.56\mathrm{e}{-5}$
Wall clock time: MLMC: 2h47m, MC (estimated): 1128h

Nonlinear constraint equation example

- Nonlinear reaction-diffusion problem

$$\begin{aligned} -\nabla \cdot (k\nabla y) + f(y) = u \quad &\text{on } D \\ y = 0 \quad &\text{on } \partial D \end{aligned}$$

- Gradient (Hessian also possible)

$$\begin{cases} -\nabla \cdot (k\nabla y) + f(y) &= u & \text{on } D \\ -\nabla \cdot (k\nabla p) + f'(y)p &= (1+\gamma)y - y_D - \gamma\mathbb{E}[y] & \text{on } D \\ \nabla \tilde{J}(u) &= 2(\alpha u + \beta \mathbb{E}[p]) \;=\; 0 & \end{cases}$$

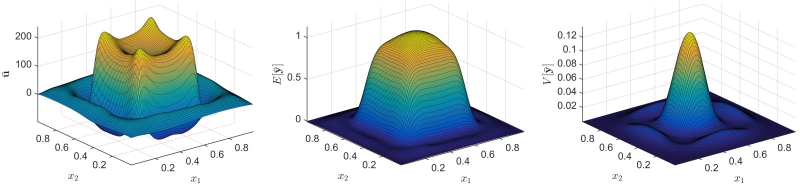
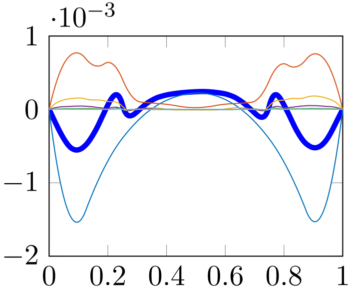
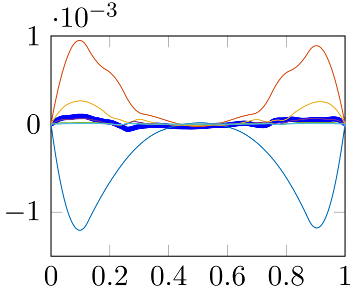


Figure: $\bar{\boldsymbol{u}}$, $\mathbb{E}[\bar{\boldsymbol{y}}]$ and $\mathbb{V}[\bar{\boldsymbol{y}}]$ for $f = e^{5y} + 20$. $\sigma^2 = 0.5$ and $n_{KL} = 250$. $\alpha = 10^{-7}$, $\gamma = 1$. 256×256 finest grid. $\tau = 5\text{e}{-5}$.

Nonlinear constraint equation example



(a) Iteration $k = 7$



(b) Iteration $k = 12$ (last)

Figure: Cross section of $\boldsymbol{g}^{(k)} = \sum_{\ell=0}^{L} I_\ell^{\bar{L}} \hat{Y}_{\ell,n_\ell}^{\mathsf{MC}}$ (——) and of contributions $I_\ell^{\bar{L}} \hat{Y}_{\ell,n_\ell}^{\mathsf{MC}}$ at levels $0, \ldots, L$ (——, ——, ——, ——, ——, ——).

Nonlinear constraint equation example

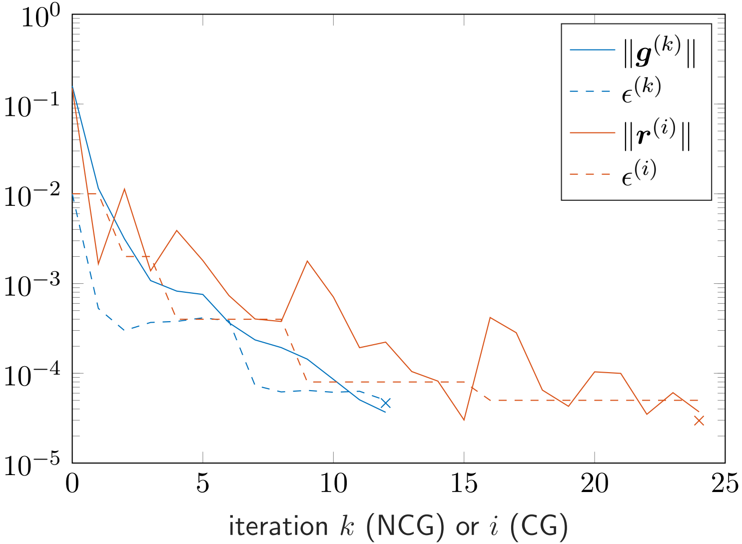


Figure: Behavior of gradient (NCG) and Hessian (CG) based optimization

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Questions?